

Abstract. – The unitary time evolution of a critical quantum spin chain with an impurity is calculated, and the entanglement evolution is shown. Moreover, we show that the reduced density matrix of a part of the chain evolves such that the fidelity of its spectrum is very high with respect to a state in thermal equilibrium. Hence, a thermal state occurs through unitary time evolution in a simple spin chain with impurity.

Thermalization through unitary evolution of pure states

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Introduction. – Systems that are left alone to evolve in interaction with an environment at a certain temperature, usually relax into a state in thermal equilibrium with its environment, and in accordance with the ergodic hypothesis, this has been shown experimentally for numerous examples in classical systems. How this happens has been the subject of intense research for many decades. The corresponding quantum case is usually viewed as a stochastic process of "quantum jumps", [1] where only the transition probabilities are calculated from the underlying unitary quantum dynamics (connected by the Fermi Golden rule). The hypotheses behind this paper, however, is that thermalization should generally occur in quantum systems describing a macroscopic world, even when all its dynamics is described by pure unitary evolution.

Quantum spin chains have been a matter of keen investigation over the latest years, and in particular their critical properties have been investigated thoroughly since it was discovered that the non-classical correlations known as entanglement are characteristic in quantum phase transitions [2]. This gives rise to the study of entanglement in the chains, in particular at critical points, as a part of the vast and expanding field of quantum information science [3]. Moreover, it has been identified that at critical points, conformal symmetry arises in a large class of models, and the characteristics of conformal field theory can be used to describe the universal properties of such systems [4]. For a certain class of models the chain can be fermionized, which makes them more accessible to analytic and numerical investigation [5]. Indeed, the propagation of entanglement is complicated [6], but can be described by conformal field theory approaches [7], and scaling laws for the entanglement have been found [8]

Any existent entanglement measured by the concurrence (*i.e.* the entanglement of formation of two spins) in the quantum spin chain at zero temperature disappears when the

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temperature of the system exceeds a threshold temperature, see e.g. [9]. However, the entanglement entropy does not vanish, indeed conformal field theory predicts that an infinitely long conformally invariant state in thermal equilibrium at temperature β has entropy proportional to the temperature at high temperatures [10]. The entropy is not an entanglement measure if the entire system is not in a pure state, such as a thermal state. The dynamics resulting in thermalization have also been discussed in other recent works [11].

In this paper we consider a quantum spin chain as sketched in Fig. 1, *i.e.* a system of N spins with open boundary conditions. The chain is initially in some arbitrary excited pure state $|\psi\rangle$ with finite excitation energy per site, and evolves according to a unitary time evolution. We trace out some part of the system, which we denote the environment, to obtain the reduced density matrix $\rho = \text{Tr}' |\psi\rangle\langle\psi|$ of the subsystem which consists of N' spins. At some spin site we introduce a magnetic impurity, that is an additional local magnetic field. In the last section of this letter we also consider what happens when the link between the system and the environment is cut. We will consider both the entropy of the state ρ , and the characteristics of ρ as related to a state in thermal equilibrium with its environment.

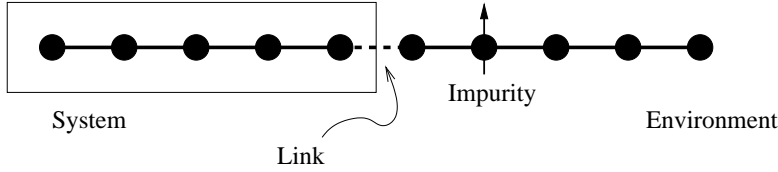


Fig. 1 – Conceptual sketch of the spin chain under consideration. Each filled circle is a spin site, and the links between them is indicated through lines. The location of the magnetic impurity is not fixed. The entire chain is in a pure state $|\psi\rangle$ while the subsystem is described by the reduced density matrix ρ .

Model. – We consider a critical Ising chain with open boundary conditions, and with a magnetic impurity at site α ,

$$\mathcal{H} = - \sum_{n=1}^N (\sigma_n^x \sigma_{n+1}^x + \sigma_n^z) + \delta \sigma_\alpha^z, \quad \sigma_{N+1}^x = 0. \quad (1)$$

Here $\sigma_n^{(x,y,z)}$ are the Pauli spin matrices at site n . $\delta \geq 0$ is the strength of the extra magnetic field at the impurity. If $\delta = 0$ we recover the critical Ising model. The impurity will destroy many of the symmetries in the system, and thereby the conservation laws, which ensures that the initial state will evolve non-trivially.

We configure the system in the initial state $|\psi_0\rangle = |\psi(t=0)\rangle$ which is not an eigenstate of the above Hamiltonian. Rather, we choose it as an excited eigenstate of the unperturbed Hamiltonian \mathcal{H}_0 . Thus it will be “almost” an eigenstate of the full Hamiltonian, and its time evolution will be nontrivial.

To the Hamiltonian (1) we apply a Jordan-Wigner transform, making it possible to map the model onto a string of fermions [12]. This amounts to defining the fermionic operators $\hat{c}_n = \frac{1}{2} \left(\bigotimes_{k=1}^{n-1} \sigma_k^z \right) \otimes (\sigma_n^x + i\sigma_n^y)$ and their adjoints, such that $\{\hat{c}_m, \hat{c}_n^\dagger\} = \delta_{mn}$. Furthermore we define the $2N$ Majorana fermions, which map two Majorana fermions onto one of the fermions defined by \hat{c}_n ,

$$\tilde{\gamma}_{2n-1} = \frac{1}{i\sqrt{2}} (\hat{c}_n - \hat{c}_n^\dagger) \quad \tilde{\gamma}_{2n} = \frac{1}{\sqrt{2}} (\hat{c}_n + \hat{c}_n^\dagger) \quad \{\tilde{\gamma}_i, \tilde{\gamma}_j\} = \delta_{ij}.$$

This diagonalizes the Hamiltonian in the sense that $\mathcal{H} = \sum_{ij} C_{ij} \tilde{\gamma}_i \tilde{\gamma}_j$ where C is an imaginary block diagonal matrix with N antisymmetric 2×2 blocks. Finally, we define the correlation matrix $\Gamma_{ij} = \langle [\tilde{\gamma}_i, \tilde{\gamma}_j] \rangle$. From this one can then trace out the physical spins intended, two adjacent rows per spin. Hence one can compute physical properties such as the entropy for the reduced density matrix. In the Heisenberg picture the time evolution of the Majorana fermions is

$$\frac{d}{dt} \tilde{\gamma}_k = i [\mathcal{H}, \tilde{\gamma}_k] = -2i \sum_i C_{ki} \tilde{\gamma}_i. \quad (2)$$

If we denote the k th element of the n th eigenvector of C as $v_k^{(n)}$ and the corresponding eigenvalue as ξ_k , the general solution of the above equation is $\tilde{\gamma}_k(t) = \mathbb{T}_{kl}(t) \tilde{\gamma}_l(0)$ with

$$\mathbb{T}_{kl}(t) = \sum_n v_k^{(n)} v_l^{(n)*} e^{-2i\xi_n t}.$$

Hence the correlation matrix evolves with time as $\Gamma(t) = \mathbb{T}(t)\Gamma(0)\mathbb{T}^T(t)$. This is our equation of motion for the state defined by Γ_{ij} . The time evolution is explicitly known, so that the correlation matrix at any time t is directly accessible and there is no accumulation of errors with time.

Entanglement evolution. – The state $|\psi(t)\rangle$ represented by the correlation matrix $\Gamma(t)$, the entanglement of one part of the system with the rest can be defined in terms of the von Neumann entropy, $S = -\text{Tr} \rho \log_2 \rho$ where $\rho = \text{Tr}' |\psi(t)\rangle \langle \psi(t)|$ amounts to tracing out some part of the system, i.e. removing the $2(N - N')$ columns and rows corresponding to the environment from $\Gamma(t)$. The reduced density matrix is diagonal in the basis of the \hat{c} fermions, and can be written

$$\rho = \prod_{k=1}^{N'} \frac{1}{1 + e^{-\omega_k}} e^{-\omega_k \hat{c}_k^\dagger \hat{c}_k}. \quad (3)$$

Here $\omega_k \in [0, \infty)$ are a set of parameters defining the state. Given that the eigenvalues of $\Gamma(t)$ are $\pm \lambda_k$ with $0 < \lambda_k < 1/2$, we find that $\lambda_k = \frac{1}{2} \tanh \frac{1}{2} \omega_k$. All states are thus defined by their N' parameters ω_k or λ_k . A pure state of the full system can also be defined by the 2^N fermionic occupation numbers in the full \hat{c} basis.

The entropy of the reduced density matrix defined by the λ_k s is now

$$S = \sum_{k=1}^{N'} H \left(\frac{1}{2} (1 + 2\lambda_k) \right) \quad (4)$$

where $H(x) = -x \log_2 x - (1 - x) \log_2 (1 - x)$ is the binary entropy function. All states in the following are written in the basis of \hat{c} fermions unless otherwise stated, that is the state is defined by a series of N binary digits, and we may for simplicity uniquely label a state by its decimal number, e.g. $|101\rangle \equiv |5_d\rangle$.

The simplest conceivable system is that of two particles, and with an impurity of strength $\delta = 1$ at one site, the entanglement entropy evolves with a simple periodic behaviour. The periodicity disappears for any larger system. Moreover, the specific choice of impurity location has a profound effect on the evolution, as shown in Fig. 2. Hence, any system larger than the trivial $N = 2$ system is very irregular in its evolution.

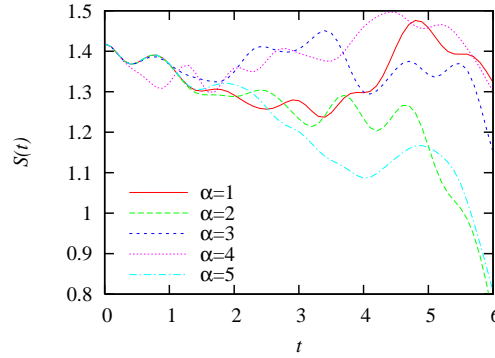


Fig. 2 – (Colour on-line) The entanglement entropy with time for a system of $N = 10$ spins where 5 spins are traced out. The initial state in all cases is $|\psi_0\rangle = |32_d\rangle$. The impurity strength is $\delta = 1$, placed at different positions α in the chain. Note that α and $N - \alpha + 1$ are equivalent positions.

Thermal states. – Next we consider a state in thermal equilibrium with its environment. Eventually, the time evolved state will be compared to the closest thermal state. A thermal state has density matrix

$$\sigma = \frac{1}{Z} e^{-\beta \mathcal{H}} = \frac{1}{Z} \sum_n e^{-\beta E_n} |\psi_n\rangle \langle \psi_n|$$

where $Z = \text{Tr} e^{-\beta \mathcal{H}}$ is the partition function, β is inverse temperature and $|\psi_n\rangle$ (E_n) are the eigenstates (-values) of the Hamiltonian \mathcal{H} . To compare the thermal state σ with some other state ρ , define the fidelity $F(\sigma, \rho) = \text{Tr} \sqrt{\sigma^{1/2} \rho \sigma^{1/2}}$ between these. The fidelity is one if the states are equal, and less otherwise. Indeed, the fidelity is a distinguishability measure that can be considered equivalent to a distance measure of mixed states [3]. However, computing the fidelity between the mixed states is computationally hard unless the density matrices commute. Hence, we will consider the classical fidelity between the eigenvalue distributions of the two density matrices, which is equal to the quantum fidelity above only in the case where they commute,

$$F_c(\sigma, \rho) = \prod_{k=1}^{N'} \frac{1 + e^{-\frac{1}{2}(\omega_k + \beta E_k)}}{\sqrt{(1 + e^{-\omega_k})(1 + e^{-\beta E_k})}} \quad (5)$$

given that E_k and ω_k both are ordered increasingly.

To compute the fidelity, we need a good estimate of the inverse temperature β . To this end, consider a state in thermal equilibrium in a canonical ensemble, which should obey the equality

$$\ln Z = S_T - \beta U. \quad (6)$$

Here, $U = -\partial \ln Z / \partial \beta$ is the internal energy and S_T is the thermodynamical entropy. The entanglement entropy is conventionally computed base two while the thermodynamic entropy is computed in the natural base, hence $S_T = S \ln 2$. We find that the equation of state (6) can be fulfilled by adjusting β until equilibrium is reached. That is, with a guess of β and the energy spectrum of the Hamiltonian, one can find $\ln Z$ in a neighborhood $\beta \pm \delta \beta$ and thus U . S_T is given by the state ρ , and by adjusting β one can now find the intersection point where (6) is fulfilled. Coincidentally, this is very close to the temperature where the fidelity

is highest, and therefore adjusting to thermal equilibrium is closely equivalent to doing a best fit to estimate β .

Given a reduced density matrix $\rho = \text{Tr}'|\psi\rangle\langle\psi|$ of a 1D system such as a spin chain in state $|\psi\rangle$, this can become thermal under time evolution in the sense that it has an eigenvalue distribution which has fidelity close to unity with a thermal state of some temperature β^{-1} . $|\psi\rangle$ cannot be an exact eigenstate of the system's Hamiltonian since this would not give rise to a time evolution. Therefore we apply the Hamiltonian (1) prepared in an initial state $|\psi_0\rangle$, which is an eigenstate of the chain with $\delta = 0$. The initial state is chosen as a state where the binary digits defining the state in the \hat{c} basis of the unperturbed Hamiltonian are chosen at random.

We consider a system of $N = 50$ spins, which allows us to investigate all eigenvalues and compare to those of a thermal state. Also, for a system of this size, the chance of a random state being close to a thermal state is negligible. In particular, we find that a randomly picked state on average has lower fidelity with a thermal state as N increases. In Fig. 3 the time evolution of the fidelity is shown for three different initial states. We see that all states quickly gains a higher fidelity, which is retained although there are some fluctuations. In Fig. 4 the eigenvalue distribution is plotted along with the thermal spectrum for the best fitted temperature for two values of t . We see clearly that the nature of the spectrum is closer to the thermal spectrum after the initialization as reflected in the fidelity.

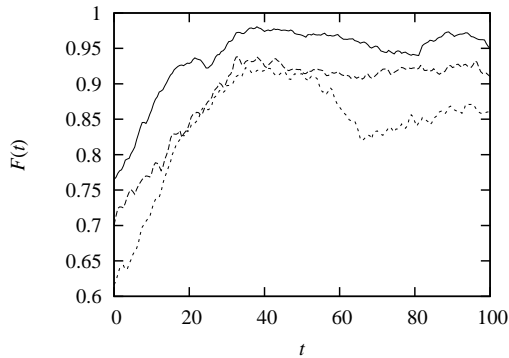


Fig. 3

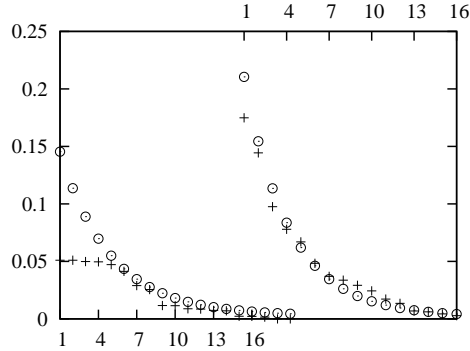


Fig. 4

Fig. 3 – The fidelity of a state with time for three different initial states and $N = 50$. The impurity is at the middle of the chain with strength $\delta = 1$. At each time step a new estimate for the temperature of the state is applied.

Fig. 4 – The eigenvalue distribution $e^{-\omega_k}$ of the reduced density matrix for the state whose time evolution is drawn with full line in Fig. 3 is plotted (+) along with the thermal distribution for a best fitted temperature (o), $e^{-\beta E_k}$. To the left are the spectra at $t = 0$ where $F = 0.77$, while to the right is the spectra for the same state after time evolution at $t = 30$ where $F = 0.96$.

To average out the random fluctuations, we define the average fidelity recorded over some time span $t_1 < t < t_2$, which we denote $\langle F \rangle$. A new guess for β is done at every time step. In Fig. 5 the average fidelity after some initializing time is plotted with the input fidelity for a selection of randomly picked states. The output state is always more thermalized than the input, in the figure indicated by the fact that all states lie above the diagonal line, except where the input state by chance already resembled a thermal state in its spectrum. However, there is some variety as to how well the states thermalize.

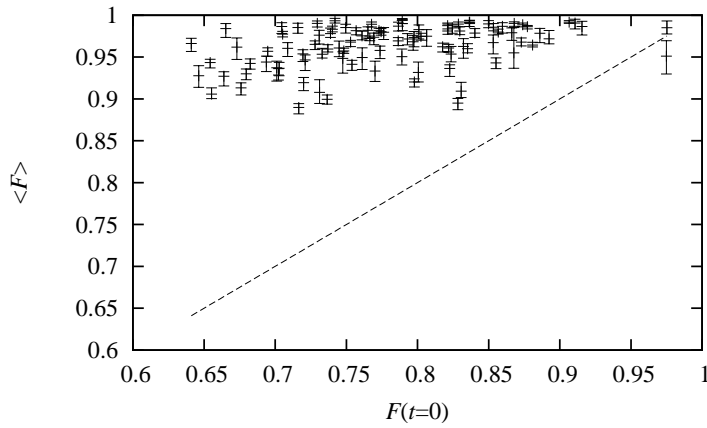


Fig. 5 – The fidelity of a random initial state with a thermal state on the x -axis and the fidelity of the state after a warmup period. The error bars indicate the range of the fidelity over the timespan recorded. Here the output state is recorded over the time $30 < t < 40$. The impurity is situated at the middle of the chain with strength $\delta = 1$ and $N = 50$. The straight line is where $\langle F \rangle = F(0)$, i.e. where there is no thermalization.

Entanglement induction. – Finally, we investigate a different type of impurity, namely a disconnection of the chain. To this end, consider the chain defined by $\mathcal{H}' = \mathcal{H} - \sigma_{N'}^x \sigma_{N'+1}^x$. The last term disconnects the chain described by the reduced density matrix ρ from its environment. Hence, there is no interaction across the boundary, and the only communication between the two sides is through the entanglement of the original state. It turns out that the single impurity of cutting the bond does not induce a thermal state in the sense that the output fidelity on average is no larger than the input fidelity. However, reinstating the magnetic impurity in addition to the decoupling of the chain makes the chain thermalize again. This confirms that the magnetic impurity is necessary to thermalize the state, though the physical coupling across the boundary is not fundamentally important. As shown in Figs. 6 and 7, the output average fidelity is close to unity (i.e. $\langle F \rangle > 0.9$) for most states even when the chain is decoupled, indeed the coupling does not seem to make much difference as to whether the chain thermalizes or not.

Thus it is clear that the entanglement present in the state has enough correlations to induce the thermalization of the state under this dynamics. A state that is a product state, $|\psi\rangle = |\psi_{\text{system}}\rangle \otimes |\psi_{\text{environment}}\rangle$ would remain a product state under Hamiltonians that do not provide interaction between the system and the environment. However there is no clear connection between how entangled the state is, as measured by the entanglement entropy, and how well it thermalizes.

Conclusion. – We have seen that the reduced density matrix of a part of a spin chain in a pure chain evolves with time such that the spectrum of the reduced state has fidelity with that of a thermal state close to unity. Thus, thermalization of a state can be achieved through simple unitary time evolution. This even holds when the link between the subsystem and its environment is cut. Then the induction of a thermal state must be caused by the entanglement correlations in the state.

The requirements on the total system is that it is sufficiently large, with a non-zero energy per degree of freedom above the vacuum energy, and that the unitary evolution is sufficiently

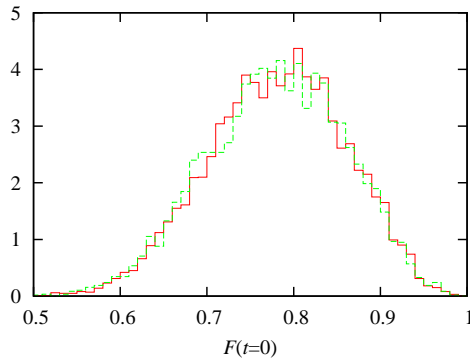


Fig. 6

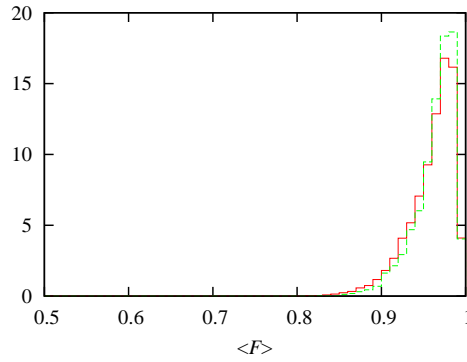


Fig. 7

Fig. 6 – (Colour on-line) A histogram of the fidelity of a random state with 10,000 samples and $N = 50$. A magnetic impurity of strength $\delta = 1$ is at mid-chain. The red line is for a normal chain, while the green line is when the chain is decoupled from its environment.

Fig. 7 – (Colour on-line) The average fidelity after a time evolution. The fidelity is averaged over time $30 < t < 40$. The states that are evolved are the same as the initial states used in Fig. 6

mixing. I.e. the wave function for the total system should not be constrained by too many conservation laws to hamper it from visiting typical regions of Hilbert space. Finally the subsystem under consideration, which we describe by a density matrix by tracing out all external degrees of freedom from the pure state, must perhaps be small compared to the total system if we want to compare its density matrix with one from a canonical or grand canonical ensemble. For this to be the case it must be that *almost all* states in the total Hilbert space, on the manifold satisfying the appropriate conservation laws, will lead to a thermal state when tracing out the external degrees of freedom. It can't be that the dynamics by miracle drive the total system towards some special states with this property.

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